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THEORETICAL STUDIES OF DETONATION WAVES

Prepared by

Stanford Research Institute
333 Ravenswood Avenue
Menlo Park, California

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US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
BALLISTIC RESEARCH LABORATORY
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Theoretical studies of reactive shock waves were performed to obtain a fundamental understanding of the initiation and propagation of detonation in condensed explosives. The differential equation governing a shock discontinuity was used to determine different conditions associated with a single shock trajectory for build-up to detonation. One of these conditions was used to construct the type of flow observed in PBX 9404 during the early stages of initiation produced by a flying plate. Various aspects of initiation induced by a constant velocity piston were considered. Equations relating the initial

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flow to the initial energy release rate were derived. Conditions were also determined for the shock to accelerate with either a positive or a negative pressure gradient. These conditions demonstrate how the mechanism of initiation depends on the energy release rate, the sound speed, and on the relationship between these quantities. A critical energy was defined for waves that build up to detonation with a positive particle velocity gradient. Work on the reactive shock problem was continued and integral relationships for unsteady flow were derived as generalized Rankine-Hugoniot equations without making approximations. Attempts to construct explicit solutions for the buildup to steady state detonation in a polytropic explosive with a prescribed energy release rate were unsuccessful. Steady detonation governed by a simple reaction rate was considered and a perturbation analysis was performed to obtain a sufficient condition for its stability.

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I INTRODUCTION

The theoretical work presented in this report was undertaken with the long-range objective of developing a better basic understanding of the initiation and propagation of detonation in condensed explosives. The achievement of this objective is necessary in a program for the improved characterization, control, and effective use of explosives in military applications. Theoretical studies are an essential part of such a program because experimental studies of detonating explosives are not completely definitive and depend on models of shock-induced reactive flow for their analysis and interpretation.

Studies of Zeldovich-von Neumann-Doering (Z-N-D) waves[1-3] were performed to elucidate and determine the parameters that govern the initiation of detonation. The problem of a single shock trajectory for buildup to detonation was considered, and the differential equation governing a shock discontinuity was examined to determine different conditions for this type of flow. One of these conditions was used to model the type of flow observed in PBX 9404 during the early stages of initiation produced by a flying plate.

Other properties of initiation produced by a constant velocity piston were considered. The equations relating the initial flow to the initial energy release rate in such a wave were derived, as well as conditions for the shock to accelerate with either a positive or a negative pressure gradient. These conditions demonstrate the dependence of the initiation process on the energy release rate, the sound speed, and the relationship between these quantities. A critical energy was defined for waves that build up to detonation with a positive pressure gradient.

Work on reactive shocks was performed with the objective of determining the dependence of initiation on the energy release rate and the rear-boundary conditions. Exact integral relationships for unsteady flow were derived as generalized Rankine-Hugoniot equations, but the attempts to construct explicit solutions for the buildup to steady detonation in a polytropic material with a prescribed energy release rate were unsuccessful.

The analysis for modeling the energy release rate in condensed explosives from Lagrange gage records obtained in shock wave experiments was extended to include integration along isochrones. This extension to the gage analysis and some results for steady detonation waves, obtained earlier[4] for Ballistic Research Laboratories, were written up as a paper entitled "Determination of Energy-Release Rate with the Hydrodynamic Properties of Detonation Waves." This paper was presented at the Fourteenth Symposium (International) on Combustion and was published in the proceedings of that meeting.

II BASIC ASSUMPTIONS

Although the basic assumptions of our theoretical studies are well defined in reference 4, they will be repeated here for completeness. Reactive shocks are treated as (Z-N-D) waves with no reaction across the shock discontinuity, and the flow induced by the shock is assumed to be adiabatic, inviscid, and in local equilibrium. Consequently, irreversible processes are restricted to shock compression and chemical reactions behind the shock.

Let e, p, and $\rho = 1/v$ denote, respectively, specific internal energy, pressure, and density--the inverse of the specific volume. Then the Rankine-Hugoniot jump conditions governing the shock discontinuity propagating into stationary material at the front of the wave can be written as:

$$\rho_H (U - u_H) = \rho_o U \tag{1}$$

$$p_H - p_o = \rho_o U u_H \tag{2}$$

$$e_H - e_o = \tfrac{1}{2}(p_H + p_o)(v_o - v_H) \tag{3}$$

where U denotes shock velocity, u denotes particle velocity, and the subscripts H and o denote quantities immediately behind and in front of the wave. Since our consideration will be restricted to rectilinear flow, it is convenient to write the conservation equations governing the flow behind the shock as:

$$\frac{1}{v}\frac{\partial v}{\partial t}\bigg|_h = \frac{\partial u}{\partial r}\bigg|_t \tag{4}$$

$$\rho_o \frac{\partial u}{\partial t}\bigg|_h = -\frac{\partial p}{\partial h}\bigg|_t \tag{5}$$

$$\frac{\partial e}{\partial t}\bigg|_h = -p\frac{\partial v}{\partial t}\bigg|_h \tag{6}$$

where h and r denote Lagrange and Eulerian distance coordinates and t denotes the time. The flow and the chemistry are coupled by the dependence of e on the reaction coordinates. For convenience in this report, only a single exothermic reaction will be considered.

Let s, T, A, and λ denote the specific entropy, temperature, the chemical affinity,[6] and the extent of reaction. Then Gibbs' equation can be written as

$$\frac{\partial e}{\partial t_h} = T \frac{\partial s}{\partial t_h} - p \frac{\partial v}{\partial t_h} - A \frac{\partial \lambda}{\partial t_h} \tag{7}$$

and the combination of Eqs. (6) and (7) gives the corresponding equation for the entropy production in shocked material as

$$T \frac{\partial s}{\partial t_h} = A \frac{\partial \lambda}{\partial t_h} \tag{8}$$

Combination of Eq. (8) with the time derivative of the $s = s(p, \rho, \lambda)$ equation of state leads to the equation

$$\frac{\partial p}{\partial t_h} = c^2 \frac{\partial \rho}{\partial t_h} + \frac{\Gamma}{v} q \frac{\partial \lambda}{\partial t_h} \tag{9}$$

where the frozen sound speed $c = (\partial p/\partial \rho)^{\frac{1}{2}}_{s,\lambda}$, the Grüneisen parameter $\Gamma/v = (\partial p/\partial e)_{v,\lambda}$, and the specific heat of reaction $q = -(\partial e/\partial \lambda)p,v$. Equation (9) is the most convenient equation for studying the interaction between the chemistry and the flow in the present treatment of Z-N-D waves. It can be derived more directly by combining Eq. (6) with the time derivative of the $e = e(p, v, \lambda)$ equation of state.

III EQUATIONS OF STATE

Equations of State of Explosives

Equations of state of condensed explosives can be constructed from the results of shock wave experiments that have been performed at the Ballistic Research Laboratories[7] and the Naval Ordnance Laboratory[8] over the last few years. These investigations lead to the conclusion that the unreacted Hugoniot curve of a condensed explosive can be adequately described by a linear relationship of the form

$$U = a + bu_H \tag{10}$$

in the $(U-u_H)$ plane. The values of the constants a and b for different explosives are given in References 7 and 8. Combination of Eq. (10) with Eqs. (1) and (2) gives the corresponding Hugoniot in the (p-v) plane as

$$p_H = \frac{a^2(v_o - v)}{[v_o - b\,(v_o - v)]^2} \tag{11}$$

and the variation of specific energy along the Hugoniot is determined by Eqs. (11) and (3). Differentiation of Eq. (11) gives the slope of the Hugoniot in the (p-v) plane as

$$\frac{dp}{dv}_H = -a^2\,\frac{[v_o + b(v_o - v)]}{[v_o - b\,(v_o - v)]^3} \tag{12}$$

and the corresponding equation for the slope of the Hugoniot in the (p-v) plane is obtained from the jump conditions as

$$\frac{dp}{du}_H = \rho_o(a + 2\,b\,u) \tag{13}$$

An expression for the sound speed along the Hugoniot $(c/v)^2_H$ in terms of $(dp/dv)_H$ can be obtained by combining the Hugoniot equation with the first and second laws of thermodynamics. Thus combination of the equations

$$\frac{de}{dv}_H = T \frac{ds}{dv}_H - p \tag{14}$$

$$\frac{de}{dv}_H = -\tfrac{1}{2}p + \tfrac{1}{2}(v_0 - v) \frac{dp}{dv}_H \tag{15}$$

$$\frac{dp}{dv}_H = -\left(\frac{c}{v}\right)^2_H + \frac{\Gamma T}{v} \frac{ds}{dv}_H \tag{16}$$

to eliminate Tds/dv_H leads to the equation

$$\left(\frac{c}{v}\right)^2_H = \frac{dp}{dv}_H \left[\frac{\Gamma}{2}\left(\frac{v_0}{v} - 1\right) - 1\right] + \frac{\Gamma}{2}\frac{p}{v} \tag{17}$$

An assumption about Γ allows the (e-p-v) equation of state of an explosive to be constructed over the volume spanned by the Hugoniot curve. If Γ is assumed to be constant, or a function of v, for example, the (e-p-v) equation of state has the form

$$e = \frac{pv}{\Gamma} + g(v) \tag{18}$$

which can be rewritten as

$$e - e_H = \frac{v}{\Gamma}\left(p - p_H\right) \tag{19}$$

since e_H and p_H are known as functions of v along the Hugoniot curve. An additional assumption about the specific heat at constant volume C_v that is consistent with $[\partial(\Gamma/v)/\partial p]_v = 0$ is then required to construct the corresponding (p-T-v) equation of state.

Equations of State of the Explosive Mixture

The equation of state of the explosive mixture will be considered in more detail because it may be necessary to remove the assumption of local thermal equilibrium at a later date.

Let the subscripts 2 and 1 denote the explosive and its products, and let the superscript 0 denote the standard state. Then the equations for the specific energy, specific entropy, and specific volume of the explosive mixture can be written as

$$e = e_2^0 - \lambda Q + \lambda e_1 + (1 - \lambda) e_2 \tag{20}$$

$$s = \lambda s_1 + (1 - \lambda) s_2 \tag{21}$$

$$v = \lambda v_1 + (1 - \lambda) v_2 \tag{22}$$

where e_2^0 denotes the heat of formation of the explosive, and $Q = e_2^0 - e_1^0$ denotes the standard heat of reaction. If e_1 and e_2 are considered to be functions of mechanical variables, then these equations of state are written formally as $e_1 = e_1(p, v_1)$ and $e_2 = e_2(p, v_2)$ with $p_1 = p_2 = p$ because the mixture is assumed to be in mechanical equilibrium. But if pressure and temperature are chosen as independent variables, they will be written as $e_1 = e_1(p, T_1)$ and $e_2 = e_2(p, T_2)$. The assumption of local thermal equilibrium is then expressed by the condition $T_1 = T_2$. Note that Eq. (10) simplifies to the equation given in reference 4,

$$e = e_2^0 - \lambda Q + \frac{pv}{\kappa - 1} \tag{23}$$

when the explosive and its products are assumed to have the polytropic equation of state with the same value of the polytropic index κ.

Combination of Eq. (6), expressing the First Law of Thermodynamics, with the time derivative of Eq. (20) leads to the equation

$$\lambda \frac{\partial e_1}{\partial t} + (1 - \lambda) \frac{\partial e_2}{\partial t} = [Q + (e_2 - e_1)] \frac{\partial \lambda}{\partial t} - p \frac{\partial v}{\partial t} \tag{24}$$

where the Lagrange subscripts have been omitted for notational simplicity. The $e_1(p, v_1)$ and $e_2(p, v_2)$ equations of state can then be used to transform the left-hand side of Eq. (24) into the expression

$$\frac{\partial p}{\partial t} \left[\lambda \left(\frac{\partial e_1}{\partial p} \right)_{v_1} + (1 - \lambda) \left(\frac{\partial e_2}{\partial p} \right)_{v_2} \right] + \left[\lambda \left(\frac{\partial e_1}{\partial v_1} \right)_p \frac{\partial v_1}{\partial t} + (1 - \lambda) \left(\frac{\partial e_2}{\partial v_2} \right) \frac{\partial v_2}{\partial t} \right] \tag{25}$$

Setting $\lambda = 0$, and $\partial v/\partial t = \partial v_2/\partial t + (v_2 - v_1)\partial\lambda/\partial t$ in Eq. (24), with the left-hand side written as shown in (25), gives the following equation for conditions at the shock front

$$\left(\frac{\partial e_2}{\partial p}\right)_{v_2}\frac{\partial p}{\partial t} + \left[\left(\frac{\partial e_2}{\partial v}\right)_p + p\right]\frac{\partial v}{\partial t} = \left[Q + (e_2 - e_1) - \left(\frac{\partial e_2}{\partial v_2}\right)_p (v_2 - v_1)\right]\frac{\partial\lambda}{\partial t} \tag{26}$$

It follows from Eq. (26) that the values of e_1 and v_1 are in general required to calculate conditions at the shock front even though the reaction is just starting. For the mixture governed by Eq. (23), however, only Q appears on the right-hand side of Eq. (26) because $e_1 = pv_1/(\kappa - 1)$, $e_2 = pv_2/(\kappa - 1)$, and $e_2 - e_1 = (\partial e_2/\partial v_2)(v_2 - v_1)$.

When $T_1 = T_2$, v_1 and v_2 can be considered as functions of v, p, and λ because the $T = T(p,v,\lambda)$ equation of state of the mixture can be formally substituted into the $v_1(T,p)$ and $v_2(T,p)$ equations of state of its constituents. In this case,

$$\frac{\partial v_1}{\partial t} = \left(\frac{\partial v_1}{\partial v}\right)_{p,\lambda}\frac{\partial v}{\partial t} + \left(\frac{\partial v_1}{\partial p}\right)_{v,\lambda}\frac{\partial p}{\partial t} + \left(\frac{\partial v_1}{\partial \lambda}\right)_{p,v}\frac{\partial \lambda}{\partial t} \tag{27}$$

$$\frac{\partial v_2}{\partial t} = \left(\frac{\partial v_2}{\partial v}\right)_{p,\lambda}\frac{\partial v}{\partial t} + \left(\frac{\partial v_2}{\partial p}\right)_{v,\lambda}\frac{\partial p}{\partial t} + \left(\frac{\partial v_2}{\partial \lambda}\right)_{p,v}\frac{\partial \lambda}{\partial t} \tag{28}$$

and Eq. (24) can be written as

$$\left(\frac{\partial e}{\partial p}\right)_{v,\lambda}\frac{\partial p}{\partial t} + \left[\left(\frac{\partial e}{\partial v}\right)_{p,\lambda} + p\right]\frac{\partial v}{\partial t} = -\left(\frac{\partial e}{\partial \lambda}\right)_{p,v}\frac{\partial \lambda}{\partial t} \tag{29}$$

with

$$\left(\frac{\partial e}{\partial p}\right)_{v,\lambda} = \lambda\left[\left(\frac{\partial e_1}{\partial p}\right)_{v_1} + \left(\frac{\partial e_1}{\partial v_1}\right)_p\left(\frac{\partial v_1}{\partial p}\right)_{v,\lambda}\right] + (1-\lambda)\left[\left(\frac{\partial e_2}{\partial p}\right)_{v_2} + \left(\frac{\partial e_2}{\partial v_2}\right)\left(\frac{\partial v_2}{\partial p}\right)_{v,\lambda}\right] \tag{30}$$

$$\left(\frac{\partial e}{\partial v}\right)_{p,\lambda} = \lambda\left(\frac{\partial e_1}{\partial v_1}\right)_p\left(\frac{\partial v_1}{\partial v}\right)_{p,\lambda} + (1-\lambda)\left(\frac{\partial e_2}{\partial v_2}\right)_p\left(\frac{\partial v_2}{\partial v}\right)_{p,\lambda} \tag{31}$$

$$\left(\frac{\partial e}{\partial \lambda}\right)_{p,v} = -\left[Q + (e_2 - e_1) - \lambda\left(\frac{\partial e_1}{\partial v_1}\right)\left(\frac{\partial v_1}{\partial \lambda}\right)_{p,v} - (1-\lambda)\left(\frac{\partial e_2}{\partial v_2}\right)_p\left(\frac{\partial v_2}{\partial \lambda}\right)_{p,v}\right] \tag{32}$$

Differentiation of Eq. (22) gives the relationship for the volume derivatives in Eq. (32) as

$$\lambda\left(\frac{\partial v_1}{\partial \lambda}\right)_{p,v} + (1 - \lambda)\left(\frac{\partial v_2}{\partial \lambda}\right)_{p,v} = -(v_1 - v_2) \qquad (33)$$

and Eq. (32) reduces to the equation $(\partial e/\partial \lambda)_{p,v} = -Q$ for the mixture satisfying Eq. (23).

IV A SINGLE SHOCK TRAJECTORY FOR BUILDUP TO DETONATION

The use of a single shock trajectory to describe the initiation of detonation in a condensed explosive was postulated by Lindstrom.[9] Lindstrom's postulate is considered here because the existence of such a single shock trajectory leads to interesting conclusions about the initiation process. Our consideration is based on the following differential equation[4] governing the pressure along the shock path

$$\left[1 + \rho_0 U\left(\frac{du}{dp}\right)_H\right]\frac{dp_H}{dt} = -\left[\rho(c^2 - (U - u)^2)\right]_H \frac{\partial u}{\partial r}_H + [\Gamma\rho q]_H \frac{\partial \lambda}{\partial t}_H \tag{34}$$

where $(du/dp)_H$ denotes the slope of the nonreactive Hugoniot curve in the (u-p) plane. It is convenient to rewrite Eq. (34) for a strong shock in material governed by Eq. (23). In this case, the mechanical jump conditions can be written as

$$U = \frac{\kappa + 1}{2} u_H \tag{35}$$

$$\rho_H = \frac{(\kappa + 1)}{(\kappa - 1)} \rho_0 \tag{36}$$

$$p_H = \frac{(\kappa + 1)}{2} \rho_0 u_H^2 \tag{37}$$

and Eq. (34) simplifies to the equation

$$\frac{dp_H}{dt} + \frac{\kappa + 1}{3} p_H \frac{\partial u}{\partial r}_H = \frac{p_D(\kappa + 1)}{6(\kappa - 1)} \frac{\partial \lambda}{\partial t}_H \tag{38}$$

where subscript D denotes the state at the front of the steady-state Chapman-Jouguet (CJ) wave, $\Gamma = (\kappa - 1)$, and q and p_D are related by the expression $(\kappa - 1)\rho_H q = (\kappa + 1)p_D/4(\kappa - 1)$.

Equation (38) cannot in general be integrated because the reactive flow is subsonic with respect to the shock, and the particle velocity gradient at the front of the wave depends on the flow between the shock and the rear boundary. There will be a unique shock trajectory in either of two cases. In the first, the particle velocity gradient at the shock front depends on a shock parameter. In the second, the piston motion, initiating the wave with initial particle velocity $u_i < u_D$, is itself generated during the buildup phase of the wave initiated with a lower initial particle velocity $u_i' < u_i$. The first case will be discussed before the second.

When the particle velocity gradient at the front of the wave depends on a shock parameter, Eq. (38) becomes an ordinary differential equation. It can then be integrated formally to give the following type of equation for the dependence of shock pressure on time,

$$p_H = p_c\, P(t/\alpha) \tag{39}$$

where p_c denotes the minimum initial pressure for the onset of detonation, $P(0) = 1$, and α is a characteristic reaction time. The introduction of a critical pressure for the onset of detonation is reasonable because many explosives are found to be nonreactive below about 40 kbar. For waves that build up to detonation, the function $P(t/\alpha)$ also satisfies the condition $P(t/\alpha) \to p_D/p_c$ as $t/\alpha \to \infty$. The relationship for shock pressure in a wave with an initial shock pressure $p_i > p_c$ can be written as

$$p_H = p_i P[(t - \tau)/\alpha] \tag{40}$$

with

$$p_i = p_c P(\tau/\alpha) \tag{41}$$

A simple solution to Eq. (38) is constructed to exemplify this type of behavior. The reaction rate along the shock path is assumed to satisfy the conditions

$$\left.\begin{aligned} \frac{\partial\lambda}{\partial t_H} &= \frac{(p_H - p_c)}{(p_D - p_c)\alpha_D} \qquad &\text{when } p_H > p_c \\ \frac{\partial\lambda}{\partial t_H} &= 0 &\text{when } p_H \le p_c \end{aligned}\right\} \tag{42}$$

It is convenient to introduce the dimensionless variables $P = p_H/p_D$ and $P_c = p_c/p_D$, and rewrite the differential equation as

$$\frac{dP}{dt} = \frac{(\kappa + 1)}{3}\left[\left(\frac{P - P_c}{1 - P_c}\right)\frac{1}{2(\kappa - 1)\alpha_D} - P\left(\frac{\partial u}{\partial r}\right)_H\right] \qquad (43)$$

It is now necessary to prescribe $(\partial u/\partial r)_H$ as a function of the shocked state to obtain a single shock trajectory. The gradient should also be prescribed so that it attains the correct value in the CJ wave. For simplicity, the particle velocity gradient was assumed to be

$$\frac{\partial u}{\partial r_H} = \frac{1}{2(\kappa - 1)\alpha_D}\,\frac{(P - P_c)}{(1 - P_c)} \qquad (44)$$

so that $(\partial u/\partial r)_H \rightarrow (\partial u/\partial r)_D$ as $P \rightarrow 1$, and the shock propagates at constant velocity when either $P_i = P_c$ or $P_i = 1$. The combination of Eqs. (43) and (44) gives the differential equation

$$\frac{(1 - P_c)}{(P - P_c)(1 - P)}\,\frac{dP}{dt} = \frac{(\kappa + 1)}{6(\kappa - 1)\alpha_D} \qquad (45)$$

which can be integrated to give

$$(P - P_c)(1 - P_i) = (P_i - P_c)(1 - P)\exp\left[(\kappa + 1)t/6(\kappa - 1)\alpha_D\right] \qquad (46)$$

Equation (46) with $\kappa = 3$ was used to plot the graph of time to detonation versus initial pressure P_i shown in Figure 1. The dimensionless time to detonation t^*/α_D was defined as the time taken for P to attain a value of 0.95.

Consider now the case when a piston initiating the flow at $p_H > p_c$ and a particle with the same initial pressure in the wave initiated at p_c follow the same path. Such a situation will occur, for example, when the acceleration of a particle depends only on its initial pressure or particle velocity. It will also occur when the acceleration is zero and the particle paths are straight lines. An exact solution for this type of flow is presented in this report because it was observed by Kennedy[10] in the early stages of initiation of detonation in PBX 9404.

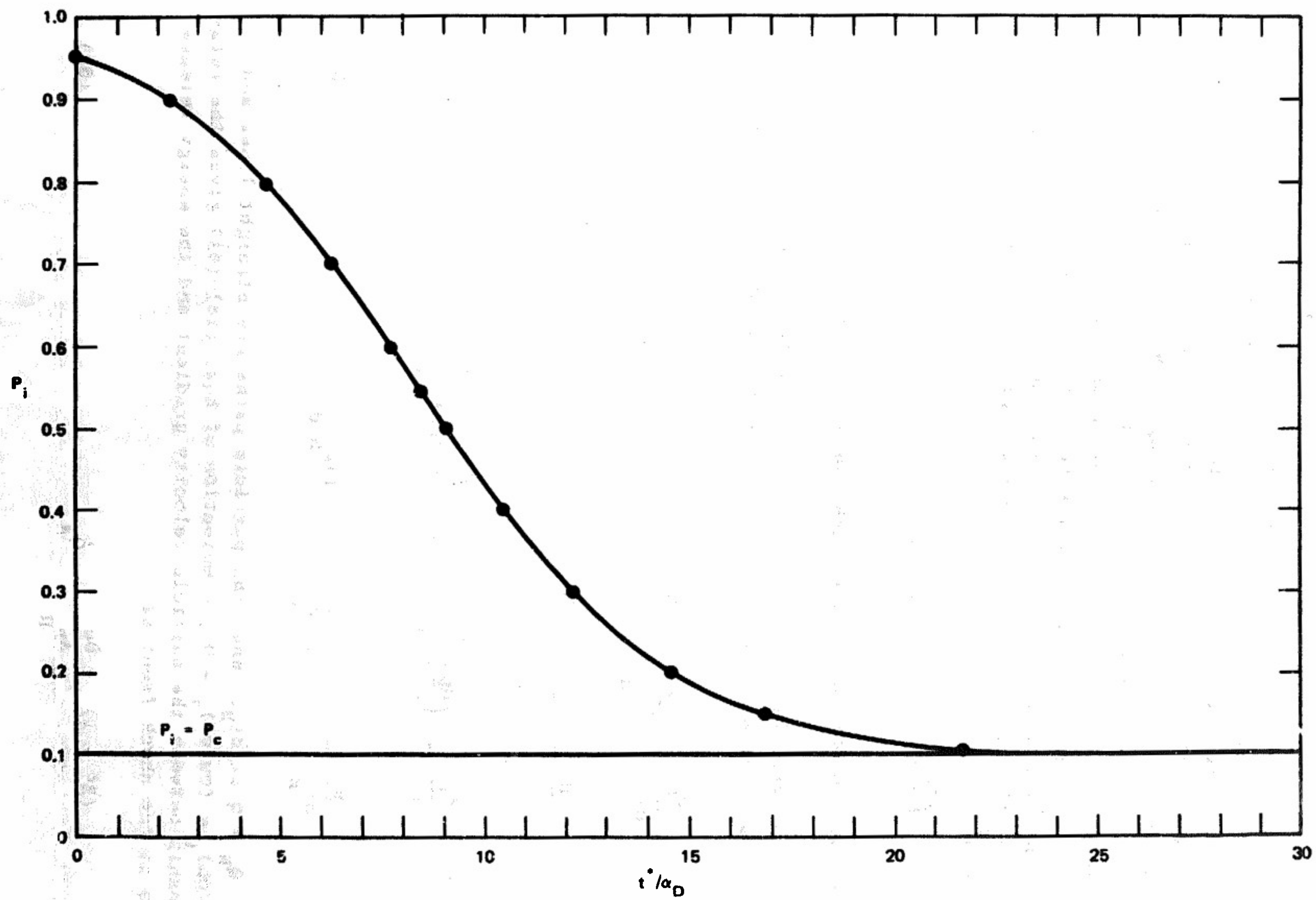

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FIGURE 1 PLOT OF TIME TO DETONATION VERSUS INITIAL PRESSURE

In these experiments, flying plates thrown at different velocities behave as constant velocity pistons and produce the same shock trajectory when the energy release rate is small. To satisfy the momentum equation, Eq. (5), the pressure must be a function only of the time t, and the particle velocity must be a function only of the Lagrange distance h. It is convenient to introduce the Lagrange time coordinate τ by the equation for the shock path $h(\tau) = \int_0^\tau U dt$, so that τ is the time a particle enters the wave and $t = \tau$ along the shock path. The shock pressure p_H and the shock particle velocity u_H can then be used to define the time dependence of the pressure and particle velocity fields as $p = p_H(t)$ and $u = u_H(\tau)$, and the Lagrange continuity equation, written as

$$\rho\left(\frac{\partial r}{\partial \tau}\right)_t = \rho_H[U(\tau) - u_H(\tau)] \tag{47}$$

can be used to obtain the corresponding density field.

The polytropic equation Eq. (23) will again be used for convenience. In this case the shock is governed by the equations

$$\frac{dp_H}{dt} = \frac{\partial p}{\partial t_H} + U\frac{\partial p}{\partial h_H} \tag{48}$$

$$\frac{du_H}{dt} = \frac{\partial u}{\partial t_H} + U\frac{\partial u}{\partial h_H} \tag{49}$$

with

$$\frac{dp_H}{dt} = \left(\frac{dp}{du}\right)_H \frac{du_H}{dt} = (\kappa - 1)(\rho u)_H \frac{du_H}{dt} \tag{50}$$

$$\frac{\partial p}{\partial t_H} = -\kappa p_H \frac{\partial u}{\partial r_H} + (\kappa - 1)\rho_H \dot{Q}_H \tag{51}$$

and $\dot{Q}_H = Q\,\partial\lambda/\partial t_H$. When the particle paths are straight lines and $(\partial p/\partial h)_t = (\partial u/\partial t)_\tau = 0$, combination of Eqs. (48)-(51) gives the relationship between the particle velocity gradient and the energy release rate at the shock front as

$$\frac{(2\kappa - 1)}{2} u_H^2 \frac{\partial u}{\partial r_H} = \dot{Q}_H \tag{52}$$

and the corresponding shock trajectory is determined by the equation

$$u_H \frac{du_H}{dt} = \frac{(\kappa - 1)}{(2\kappa - 1)} \dot{Q}_H \tag{53}$$

Integrating Eq. (53) gives the particle velocity field as

$$u(\tau) = u_i [1 + K_1 \ I(\tau)]^{\frac{1}{2}} \tag{54}$$

and the pressure field follows from the jump conditions as

$$p(t) = p_i [1 + K_1 \ I(t)] \tag{55}$$

where $K_1 = 2(\kappa - 1)/(2\kappa - 1)$, $u_i^2 \ I(\tau = t) = \int_0^{\tau=t} \dot{Q}_H(s')ds'$, and the subscript i denotes the initial condition at $t = \tau = 0$. Differentiating Eq. (54) gives the Lagrange particle velocity gradient as

$$\frac{\partial u}{\partial \tau} = \frac{K_1}{2} \frac{\dot{Q}_H(\tau)}{u(\tau)} \tag{56}$$

integrating Eq. (56) gives the deformation gradient as

$$\frac{\partial r}{\partial \tau} = \frac{1}{2} \left[\frac{(\kappa - 1)u_H^2(\tau) + K_1\dot{Q}_H(\tau)(t - \tau)}{u(\tau)} \right] \tag{57}$$

and the Eulerian particle velocity gradient follows from Eqs. (56) and (57) as

$$\frac{\partial u}{\partial t} = \frac{K_1\dot{Q}_H(\tau)}{(\kappa - 1)u_H^2(\tau) + K_1\dot{Q}_H(\tau)(t - \tau)} \tag{58}$$

Equation (57) and the Lagrange continuity equation give the equation for the specific volume as

$$v = v_H \left[1 + \frac{K_1\dot{Q}_H(\tau)(t - \tau)}{(\kappa - 1)u_H^2(\tau)} \right] \tag{59}$$

It follows from Eq. (53), (54), (55), and (59) that the energy release rate at the shock front $\dot{Q}_H$ determines the flow. The case when the

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particle velocity gradient is a function of time is of particular interest and will be considered in more detail. Equation (58) gives the condition for this type of flow as

$$(\kappa - 1)u_H^2(\tau) - K_1\dot{Q}_H(\tau)(\tau + \alpha) = 0 \tag{60}$$

where α is a characteristic time defined by the initial reaction rate, and the corresponding equations for the particle velocity gradient and the shock particle velocity follow from Eqs. (58), (60), and (53) as

$$\frac{\partial u}{\partial r} = \frac{1}{t + \alpha} \tag{61}$$

and

$$\frac{du_H}{d\tau} = \frac{(\kappa - 1)}{2} \frac{u_H}{(\tau + \alpha)} \tag{62}$$

Integration of Eq. (62) gives the particle velocity field as

$$\frac{u}{u_i} = \left[\frac{\tau + \alpha}{\alpha}\right]^{\frac{\kappa-1}{2}} \tag{63}$$

the pressure field as

$$\frac{p}{p_i} = \left[\frac{t + \alpha}{\alpha}\right]^{\kappa-1} \tag{64}$$

and the density field follows from Eq. (59) as

$$\frac{\rho}{\rho_H} = \left[\frac{\tau + \alpha}{t + \alpha}\right] \tag{65}$$

The energy equation

$$\frac{\partial p}{\partial t} = -\kappa p \frac{\partial u}{\partial r} + (\kappa - 1)\rho\dot{Q} \tag{66}$$

obtained by setting $c^2 = \kappa p/\rho$ and $\Gamma q = (\kappa - 1)Q$ in Eq. (9), gives the volumetric energy release rate as

$$\rho\dot{Q} = \frac{(2\kappa - 1)}{(\kappa - 1)} \frac{p_i}{\alpha} \left(\frac{p}{p_i}\right)^{\frac{\kappa-2}{\kappa-1}} \tag{67}$$

Since the shock pressure and particle velocity increase with time, Eqs. (63), (65) and (67) cannot be used to describe the whole of the initiation process resulting in a steady detonation wave. Other equations must therefore be patched to them to describe the approach to the steady state. It is reasonable to assume that reaction in the early stages of initiation occurs in hot spots arising from inhomogeneities. Then the energy release rate in hot spots produced at the shock front determines the flow, and the associated energy release rate behind the accelerating shock will enhance reaction in the bulk of the shocked material. If, moreover, there is a critical temperature for the onset of thermal explosion, the temperature distribution in the wave will determine where shocked material explodes and produces a second shock, which initiates bulk reaction and dominates the flow in the later stages of the initiation process.

Consider, for example, the simple case when $(\partial T/\partial\lambda)_{p,v} = (\partial p/\partial\lambda)_{T,v} = 0$, $(\partial e/\partial\lambda)_{p,v} = (\partial e/\partial\lambda)_{T,v}$, and the time rate of change of temperature along a particle path and the Lagrange temperature gradient are governed by the equations,

$$\frac{\partial T}{\partial t} = \frac{C_v(\kappa - 1)}{v}\frac{\partial p}{\partial t} + \left(\frac{\partial T}{\partial v}\right)_{p,\lambda}\frac{\partial v}{\partial t} \tag{68}$$

and

$$\frac{\partial T}{\partial \tau} = \left(\frac{\partial T}{\partial v}\right)_{p,\lambda}\frac{\partial v}{\partial \tau} \tag{69}$$

Combining Eqs. (68) and (69), subject to the condition $(\partial v/\partial t)_H = -(\partial v/\partial \tau)_H$ along the shock path, gives the equation governing the shock temperature as

$$\frac{dT_H}{dt} = \frac{C_v(\kappa - 1)}{v}\frac{dp_H}{dt} \tag{70}$$

since $\partial p/\partial t = dp_H/dt$. Since $\partial v/\partial t > 0$ it follows from Eqs. (68) and (70) that the temperature increases faster along a particle path than along the shock path. The mechanism of initiation will resemble that observed in nitromethane[11] when the initial pressure is about 80 kbar, because the critical temperature will be attained and thermal explosion will occur behind the first shock. The position where the second shock is formed, however, depends on the temperature distribution and can be determined when the explicit form of the $p = p(v,T)$ equation of state is known.

V INITIATION BY A CONSTANT VELOCITY PISTON

Initiation by a constant velocity piston was considered because flying plates are used in experimental initiation studies and because constant particle velocity is chosen as the rear boundary in many numerical studies. The problem is to understand and quantitatively account for the observed shock trajectories in condensed explosives. Of particular interest is the case when the initial shock pressure is low and the shock propagates at essentially its initial velocity before accelerating very rapidly to attain the detonation velocity. Since the wave can develop initially with either a positive or a negative pressure gradient but must have a positive gradient in the final buildup to detonation, our approach was to determine a condition for the initial shape of the wave and then look for a criticality condition for the onset of detonation. It is convenient first to derive the initial conditions in a wave initiated by a piston with an arbitrary motion. The combination of Eqs. (48)-(50) with Eq. (9) evaluated at the shock front gives the following equation for the derivatives of the particle velocity along the shock path:

$$\left[\left(\frac{dp}{du}\right)_H + \frac{U}{v_0}\right]\frac{\partial u}{\partial t_H} + \left[\left(\frac{c}{v}\right)^2 v_0 + U\frac{dp}{du_H}\right]\frac{\partial u}{\partial h_H} = \frac{\Gamma}{v}\, q\, \frac{\partial \lambda}{\partial t_H} \tag{71}$$

It follows from the momentum equation, Eq. (5), that Eq. (71) is also an equation relating the pressure and particle velocity gradients at the shock front. The initial particle velocity gradient in a wave initiated by a constant velocity piston is obtained by setting $\partial u/\partial t_H = 0$ in Eq. (71) as

$$\frac{\partial u}{\partial h_H} = \frac{\Gamma \dot{q}_H}{v[U(dp/du)_H + v_0(c/v)^2]} \tag{72}$$

where $\dot{q}_H = q\, \partial\lambda/\partial t_H$. When $(\partial u/\partial h)_H$ is known, the initial time rate of change of pressure in the wave and the initial time rate of change of shock particle velocity can be evaluated with the equations

$$\frac{dp_H}{dt} = \frac{\partial p}{\partial t_H} = U\frac{dp}{du_H}\frac{\partial u}{\partial h_H} \tag{73}$$

and

$$\frac{du_H}{dt} = U \frac{\partial u}{\partial h_H} \tag{74}$$

obtained by combining Eqs. (48)-(50) with the boundary condition $\partial u/\partial t = \partial p/\partial h = 0$. The corresponding value of the volume gradient can be evaluated with the equation,

$$\frac{\partial v}{\partial h_H} = \left[\frac{dv}{du_H} - \frac{v_o}{U}\right] \frac{\partial u}{\partial h_H} \tag{75}$$

obtained by combining the continuity equation with the identity

$$\frac{dv}{du_H} \frac{du_H}{dt} = \frac{\partial v}{\partial t_H} + U \frac{\partial v}{\partial h_H} \tag{76}$$

It follows from Eqs. (72)-(75) that the initial values of the first derivatives of the flow in a reactive wave initiated by a constant velocity piston are determined by the initial shock strength, the equation of state of the explosive, and the initial value of the energy release rate. Alternatively, a knowledge of the initial value of one of the derivatives is sufficient to determine the initial value of the energy release rate when a, b, and Γ are known. Measurement of one of these quantities in a series of experiments using flying plates thrown at different velocities is therefore sufficient to determine the dependence of the initial energy release rate on pressure.

We will now derive the equations that determine the shape of the wave during the early stages of the initiation process. For notational convenience, the subscript H will now be omitted from the derivatives, but it should be remembered that the equations specify the initial conditions in the wave. Since the piston moves with constant velocity, it follows from the momentum equation that the pressure gradient at the piston is zero. Consequently, the initial rates of change of pressure along the piston and along the shock path are equal as shown by Eq. (73), and it is necessary to find the second derivative $(\partial^2 p/\partial h^2)$ to determine whether the wave develops with a positive or a negative pressure gradient. During the early stages of the flow, the wave will develop with a positive gradient and the pressure will be higher at the shock than at the piston when the initial value of $\partial^2 p/\partial h^2 > 0$; when $\partial^2 p/\partial h^2 < 0$, the wave will develop with a negative gradient and the pressure will be

higher at the piston than at the shock; when $\partial^2 p/\partial h^2 = 0$, there will be no gradient.

The equation for $(\partial^2 p/\partial h^2)$ is derived from Eqs. (4), (5), (9), and Eqs. (48-50). Combination of the equations obtained by differentiating Eqs. (4), (5), and (9) to eliminate the second derivatives of shock pressure and particle velocity leads to the equation

$$\dot{U}\frac{\partial^2 p}{\partial h^2}\left(U + 2v_0\frac{dp}{du}\right) = -\frac{\partial^2 p}{\partial t^2} + \frac{dp}{du}\left(U^2\frac{\partial^2 u}{\partial h^2} + \frac{\partial u}{\partial h}\frac{dU}{dt}\right) + \frac{d^2 p}{du^2}\left(\frac{du_H}{dt}\right)^2 \tag{77}$$

when account is taken of the equations

$$\frac{\partial^2 u}{\partial h \partial t} = -v_0\frac{\partial^2 p}{\partial h^2} \tag{78}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 p}{\partial t \partial h} = 0 \tag{79}$$

imposed by the rear boundary condition. Partial differentation of Eq. (9) written in terms of $\partial u/\partial h$, with respect to t and h, yields expressions for $\partial^2 p/\partial t^2$ and $\partial^2 u/\partial h^2$. Substitution of these expressions into Eq. (77) then gives the required expression for $\partial^2 p/\partial h^2$.

The equation obtained for $\partial^2 p/\partial t^2$ is

$$\frac{\partial^2 p}{\partial t^2} = \left(\frac{cv_0}{v}\right)^2\frac{\partial^2 p}{\partial h^2} - v_0\frac{\partial u}{\partial h}\frac{\partial}{\partial t}\left(\frac{c}{v}\right)^2 - \Gamma\left(\frac{v_0}{v}\right)^2 v_0\frac{\partial u}{\partial h}\dot{q} + \frac{\Gamma}{v}\ddot{q} \tag{80}$$

and the equation obtained for $\partial^2 u/\partial h^2$ is

$$\frac{\partial^2 u}{\partial h^2} = -\left(\frac{v}{c}\right)^2\frac{\partial u}{\partial h}\frac{\partial}{\partial h}\left(\frac{c}{v}\right)^2 + \left(\frac{v}{c}\right)^2\Gamma\left[\left(\frac{v_0}{v}\right)\frac{1}{v_0^2}\frac{\partial \dot{q}}{\partial h} - \frac{1}{v^2}\frac{\partial v}{\partial h}\frac{\dot{q}}{v_0}\right] \tag{81}$$

The combination of Eqs. (70), (80), and (81) to eliminate $\partial^2 p/\partial t^2$ and $\partial^2 u/\partial h^2$ give the equation for $\partial^2 p/\partial h^2$ as

$$B \frac{\partial^2 p}{\partial h^2} = \frac{\partial u}{\partial h}\left[v_o \frac{\partial}{\partial t}\left(\frac{c}{v}\right)^2 - v_o^2 \frac{dp}{du}\left(\frac{vU}{v_o c}\right)^2 \frac{\partial}{\partial h}\left(\frac{c}{v}\right)^2 + \frac{dp}{du}\frac{dU}{dt} + U \frac{d^2 p}{du^2}\frac{du_H}{dt}\right]$$

$$+ \frac{\Gamma \dot{q}}{v_o}\left[\left(\frac{v_o}{v}\right)^2 \frac{\partial u}{\partial h} - \frac{dp}{du}\left(\frac{U}{c}\right)^2 \frac{\partial v}{\partial h}\right] \qquad (82)$$

$$+ \frac{\Gamma}{v}\left[\frac{dp}{du}\left(\frac{vU}{v_o c}\right)^2 v_o \frac{\partial \dot{q}}{\partial h} - \ddot{q}\right]$$

where

$$B = [U^2 + 2Uv_o dp/du + (v_o c/v)^2]$$

Equation (82) specifies the dependence of the initial shape of the pressure profile produced by a constant velocity piston on the energy release rate and the $e = e(p, v, \lambda)$ equation of state, and can be used to determine whether the wave develops with a negative or a positive pressure gradient when these quantities are known.

Consider the case when the explosive is described by Eq. (18), the products obey a polytropic equation of state, and Eq. (20) gives the $e = e(p, v, \lambda)$ equation of state as

$$e = e_2^0 - \lambda Q + \frac{pv}{K - 1} + (1 - \lambda)[K_2 p v_2 + g(v_2)] \qquad (83)$$

with $K_2 = (\Gamma^{-1} - (K - 1)^{-1})$. Note that Eq. (83) reduces to Eq. (23) when the explosive is assumed to have a polytropic equation of state since then $K_2 = g(v_2) = 0$. Equation (82) can be used to derive expressions for the derivatives $\partial(c/v)^2/\partial t$ and $\partial(c/v)^2/\partial h$ that are needed to determine the sign of $\partial^2 p/\partial h^2$. The simplest case with the explosive and its products in thermal equilibrium $(T_1 = T_2 = T)$ was considered so that the identity

$$\left(\frac{c}{v}\right)^2 = \frac{p + (\partial e/\partial v)_{p\lambda}}{(\partial e/\partial p)_{v,\lambda}} \qquad (84)$$

could be used. It is clear that the second derivatives $(\partial^2 e/\partial p^2)_{\lambda=0}$, $(\partial^2 e/\partial p \partial v)_{\lambda=0}$, $(\partial^2 e/\partial v^2)_{\lambda=0}$, $(\partial^2 e/\partial \lambda \partial p)_{\lambda=0}$, and $(\partial^2 e/\partial \lambda \partial v)_{\lambda=0}$ must be calculated in order to calculate the derivatives of $(c/v)^2$ from Eq. (84). Differentiation of Eq. (82) leads to the following equations for these derivatives

$$\left(\frac{\partial^2 e}{\partial p^2}\right)_{\lambda=0} = 0 \tag{85}$$

$$\left(\frac{\partial^2 e}{\partial p \partial v}\right)_{\lambda=0} = \frac{1}{\Gamma} \tag{86}$$

$$\left(\frac{\partial^2 e}{\partial v^2}\right)_{\lambda=0} = \frac{d^2 g}{dv_2^2} \tag{87}$$

$$\left(\frac{\partial^2 e}{\partial \lambda \partial p}\right)_{\lambda=0} = K_2(v_2 - v_1) - \left[\left(\frac{\partial v_1}{\partial p}\right)_T + \left(\frac{\partial v_1}{\partial T}\right)_p \left(\frac{\partial T}{\partial p}\right)_{v_2}\right]\left(K_2 p + \frac{dg}{dv_2}\right) \tag{88}$$

$$\left(\frac{\partial^2 e}{\partial \lambda \partial v}\right)_{\lambda=0} = \frac{d^2 g}{dv_2^2}\left(v_2 - v_1\right) - \left(\frac{\partial v_1}{\partial T}\right)_p \left(\frac{\partial T}{\partial v_2}\right)_p \left(K_2 p + \frac{dg}{dv_2}\right) \tag{89}$$

Equations (88) and (89) define the influence of the reaction on the sound speed when the explosive and its products satisfy Eq. (83). Furthermore, it follows that Eq. (83) is in general insufficient to calculate $\partial^2 p/\partial h^2$ when the energy release rate is known. Values of $\partial^2 p/\partial h^2$ based on additional equation of state assumptions were calculated and will be discussed later. But most attention was given to the simple case when the explosive is polytropic and the sound speed is not influenced by the reaction because all the second derivatives of the energy in Eqs. (85)-(89) vanish except $\partial^2 e/\partial p \partial v = 1/(\kappa - 1)$.

Evaluation of the terms in Eqs. (81) and (82) using Eq. (23) gives the following equations

$$u_1^2 \frac{\partial^2 u}{\partial h^2} = \frac{2}{\kappa}\left[\frac{(\kappa - 1)}{(\kappa + 1)}\frac{\partial \dot{Q}}{\partial h} + u_1\left\{\frac{2(\kappa - 1)}{(2\kappa - 1)(\kappa + 1)}\left(\frac{\dot{Q}}{u_1^2}\right)\right\}^2\right] \tag{90}$$

$$B\frac{\partial^2 p}{\partial h^2} = \frac{p_1 Q}{\kappa u_1^2}\left[\frac{4(\kappa^2 - 1)Q}{(2\kappa - 1)u_1^2}\left(\frac{\partial \lambda}{\partial t}\right)^2 + (\kappa^2 - 1)u_1\frac{\partial^2 \lambda}{\partial t \partial h} - 2\kappa\frac{\partial^2 \lambda}{\partial t^2}\right] \tag{91}$$

with $B = (7\kappa - 5)(\kappa + 1)^2 u_1^2/4(\kappa - 1)$, for the initial values of the second derivatives of particle velocity and pressure with respect to Lagrange distance. When the reaction rate in polytropic explosive is known as a function of state variables, Eq. (91) can be used to

determine whether the wave produced by a constant velocity piston develops initially with a positive or a negative pressure gradient.

The validity of Eq. (91) was first tested by checking that $\partial^2p/\partial h^2 = 0$ when the energy release rate is defined by Eq. (67) and the flow develops as a step shock in pressure. The expression for $\partial^2p/\partial h^2$ as calculated with

$$\frac{\partial\lambda}{\partial t} = \frac{(2\kappa - 1)}{(\kappa - 1)} \frac{p_i v}{Q\alpha} \left(\frac{p}{p_i}\right)^n \tag{92}$$

showed indeed that $\partial^2p/\partial h^2 = 0$ when $n = (\kappa - 2)/(\kappa - 1)$, and also led to the conclusion that $\partial^2p/\partial h^2 < 0$ when $n > (\kappa - 2)/(\kappa - 1)$ and that $\partial^2p/\partial h^2 > 0$ when $n < (\kappa - 2)/(\kappa - 1)$.

Expressions for $\partial^2p/\partial h^2$ were also derived using the following reaction rate laws:

$$\frac{\partial\lambda}{\partial t} = A_1 e^{-Ta/T}(1 - \lambda) \tag{93}$$

$$\frac{\partial\lambda}{\partial t} = A_2 e^{-pa/p}(1 - \lambda)^n \tag{94}$$

$$\frac{\partial\lambda}{\partial t} = A_3(1 - \lambda)^n(p - p_c)^m \tag{95}$$

Equation (93) is the well-known Arrhenius expression for a unimolecular reaction, and Eqs. (94) and (95) were used by Harper[12] and Bernier[13] to simulate the initiation behavior of condensed explosives. The form of Eq. (91) for the Arrhenius rate law will not be given here because the initiation process does not depend on the shape of the pressure profile. That this is so follows from the equations governing the temperature T. Since the volume is constant along the shock path, the rates of change of temperature and pressure at the shock front are related by the equation

$$\left(\frac{\partial p}{\partial T}\right)_{v,\lambda} \frac{dT_H}{dt} = \frac{dp_H}{dt} \tag{96}$$

The rates of change of temperature and pressure along a particle path, however, are related by the equation

$$\left(\frac{\partial p}{\partial T}\right)_{v,\lambda} \frac{\partial T}{\partial t} = \frac{\partial p}{\partial t} + \rho c^2 \frac{C_{v,\lambda}}{C_{p,\lambda}} \left(\frac{\partial u}{\partial h}\right)\left(\frac{\partial h}{\partial r}\right) \qquad (97)$$

where $C_{v,\lambda}$ and $C_{p,\lambda}$ denote the specific heats at constant volume and pressure. Initially therefore when $dp_H/dt = \partial p/\partial t$, $\partial T/\partial t > dT_H/dt$ and $\partial T/\partial h < 0$, the temperature will increase faster along the piston path than along the shock path. As a consequence, the reaction rate will be highest at the piston for both a positive and a negative pressure gradient. The criticality condition for initiation is then that the piston motion be maintained for a time longer than the characteristic reaction time

$$t_c = \frac{A_1^{-1} T_i^2 C_{v,\lambda} e^{T_a/T_i}}{T_a Q} \qquad (98)$$

when $T_a/T_i \gg 1$ and T_i denotes the initial shock temperature.

The situation is different for a pressure-dependent energy release rate because then the mechanism of initiation depends on the initial shape of the pressure pulse. Consider first the case when the initial value of $\partial^2 p/\partial h^2 < 0$. The pressure and reaction rate will increase faster along the piston path than along the shock path, and the wave will build up initially from behind. But when $\partial^2 p/\partial h^2 > 0$, the pressure and reaction rate will increase faster along the shock path than along a particle path, and the wave will build up at the front. Since $\partial p/\partial h > 0$ in the steady wave, however, the initiation of detonation will exhibit both types of flow when the initial value of $\partial^2 p/\partial h^2 < 0$. Buildup to detonation in high density PETN exhibiting $\partial p/\partial h < 0$ and $\partial p/\partial h > 0$ was recently observed by Wackerle and Johnson.[14] As the initial pressure is increased, the mechanism of initiation will change from one involving a negative and positive pressure gradient to one involving only a positive pressure gradient. To be more specific, consider the cases when the energy release rate is governed by Eqs. (94) and (95), and Eq. (91) becomes

$$B\left(\frac{\partial^2 p}{\partial h^2}\right) = \frac{p_i Q\, 4(\kappa - 1)}{u_i^2 (2\kappa - 1)} \left(\frac{\partial \lambda}{\partial t}\right)_i^2 \left[\left(\frac{\kappa + 1}{\kappa} - \frac{p_a}{p_i}\right)\frac{Q}{u_i^2} + \frac{(2\kappa - 1)^2 n}{2\kappa(\kappa - 1)}\right] \qquad (99)$$

and

$$B\left(\frac{\partial^2 p}{\partial h^2}\right) = \frac{p_i Q 2(\kappa - 1)}{u_i^2 (2\kappa - 1)} \left(\frac{\partial \lambda}{\partial t}\right)_i^2 \left[2\left(\frac{(\kappa + 1)}{\kappa} - \frac{m}{1 - p_c/p_i}\right)\frac{Q}{u_i^2} + \frac{(2\kappa - 1)^2 n}{\kappa(\kappa - 1)}\right]. \qquad (100)$$

Equation (99) shows that $\partial^2 p/\partial h^2 < 0$ when $p_a/p_i \gg 1$. When $\partial\lambda/\partial t$ is small, the energy release rate is highest at the piston, and the criticality condition for initiation is that the piston motion be maintained for a time longer than the characteristic reaction time

$$t_c = A_2^{-1} \frac{p_i^2 v_i e^{p_a/p_i}}{p_a \Gamma Q} . \tag{101}$$

Equation (100) shows that $\partial^2 p/\partial h^2 > 0$ when the initial pressure is less than p_i defined by the condition $1 - p_c/p_i = (\kappa + 1)/\kappa m$. When this condition is satisfied, the wave will build up to detonation with a positive pressure gradient as shown by the results of Bernier's numerical calculations.[13] This type of buildup should also be observed in the former case when $p_a/p_i \approx 1$.

Calculations of the initial values of $\partial^2 p/\partial h^2$ at various shock velocities and pressures were performed using pressure-dependent energy release rates; a general equation of state in which the unreacted explosive has a Hugoniot curve of the form $U = a + bu_H$ and the detonation product gases have a polytropic equation of state; and the detonation properties of PBX 9404-03, case Composition B-3, and cast TNT. For all three explosives the initial values of $\partial^2 p/\partial h^2$ are negative at low initial shock velocities and then become positive at higher shock velocities. The change in sign of $\partial^2 p/\partial h^2$ occurs at a shock velocity significantly below the detonation velocity for PBX 9404-03, and at a shock velocity significantly higher than the detonation velocity for cast TNT. The shock velocity at which the initial value of $\partial^2 p/\partial h^2$ becomes positive thus increases as the sensitivity of the solid explosive to shock initiation decreases. Since $\partial^2 p/\partial h^2$ remains negative for initial shock velocities exceeding the steady state detonation velocity in cast TNT, the calculations predict the formation of a reactive pressure pulse at the piston face; this pulse eventually overtakes the initial shock front and causes detonation. This type of initiation has been observed in homogeneous liquid explosives and in high density PETN and XTX-8003. The buildup to detonation in PBX 9404-03 and Composition B-3 is typical of heterogeneous solid explosives in which the initial shock front is strengthened and accelerated without the appearance of a velocity overshoot.

Smooth buildup to detonation with $(\partial^2 p/\partial h^2)_i > 0$, resulting from the impact of a flying plate, will now be discussed. For convenience,

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the flow is assumed to satisfy the condition $\partial^2 p/\partial h^2 > 0$ so that $\partial^2 u/\partial h \partial t < 0$, and the pressure on the piston is assumed to attain a maximum during the course of the reaction. The relationship between the particle velocity gradient and the energy release rate when the pressure on the piston is a maximum is obtained by setting $\partial p/\partial t = 0$ in the energy equation, rewritten as

$$\frac{\partial r}{\partial h}\frac{\partial p}{\partial t} = -\frac{c^2}{v}\frac{\partial u}{\partial h} + \frac{\Gamma}{v_0} q \frac{\partial \lambda}{\partial t} . \qquad (102)$$

The particle velocity gradient on the piston is also assumed to be positive during the course of the reaction. The curves of constant pressure were sketched to gain a better understanding of this type of flow, and a critical energy was defined for the initiation of detonation.

Since $\partial^2 p/\partial h^2 > 0$ at the piston, the pressure increases faster along the shock path than along the piston path, and the flow develops with a positive pressure gradient. The curves of constant pressure in the (t-h) plane for such a flow are shown schematically in Figure 2 where OCS represents the shock path, ODP represents the piston path, and DC represents the locus of pressure peaks.

Particles that enter the wave before t_c attain their maximum pressure along DC, but particles that enter the wave after t_c attain their maximum pressure at the shock front. Qualitative features of the curves of constant pressure follow directly from the identity

$$\frac{\partial p}{\partial t} = -C_p \frac{\partial p}{\partial h} \qquad (103)$$

where $C_p = (\partial h/\partial t)_p$ denotes the slope of a curve of constant pressure. We are interested in the case when $\partial p/\partial h \geq 0$. When $\partial p/\partial h > 0$, the sign of C_p is determined by the time rate of change of pressure along a particle path, and $C_p < 0$ where $\partial p/\partial t > 0$, but $C_p > 0$ where $\partial p/\partial t < 0$. When $\partial p/\partial h = 0$, however, $(\partial t/\partial h)_p = 0$ where $(\partial p/\partial t) \neq 0$, and

$$C_p = \left(-\frac{\partial^2 p/\partial t^2}{\partial^2 p/\partial h^2}\right)^{\frac{1}{2}} \qquad (104)$$

at a singular point where $\partial p/\partial t = 0$. We are now in a position to consider the curves of constant pressure emanating from the piston. Since $\partial p/\partial h = 0$ at the piston, the curves of constant pressure intersect the

piston path at right angles except at the singular point D where $\partial p/\partial t = 0$. The curves emanating from the piston before t_d have negative slopes and intersect the shock path because the pressure is higher at the shock than at the piston. But the curves emanating from the piston after t_d have positive slopes and do not intersect the shock path because the pressure is decreasing along a particle path while it is increasing along the shock path. When $\partial^2 p/\partial t^2 < 0$ at D, D is a double point, and the slopes of the curves passing through it are determined by Eq. (104).

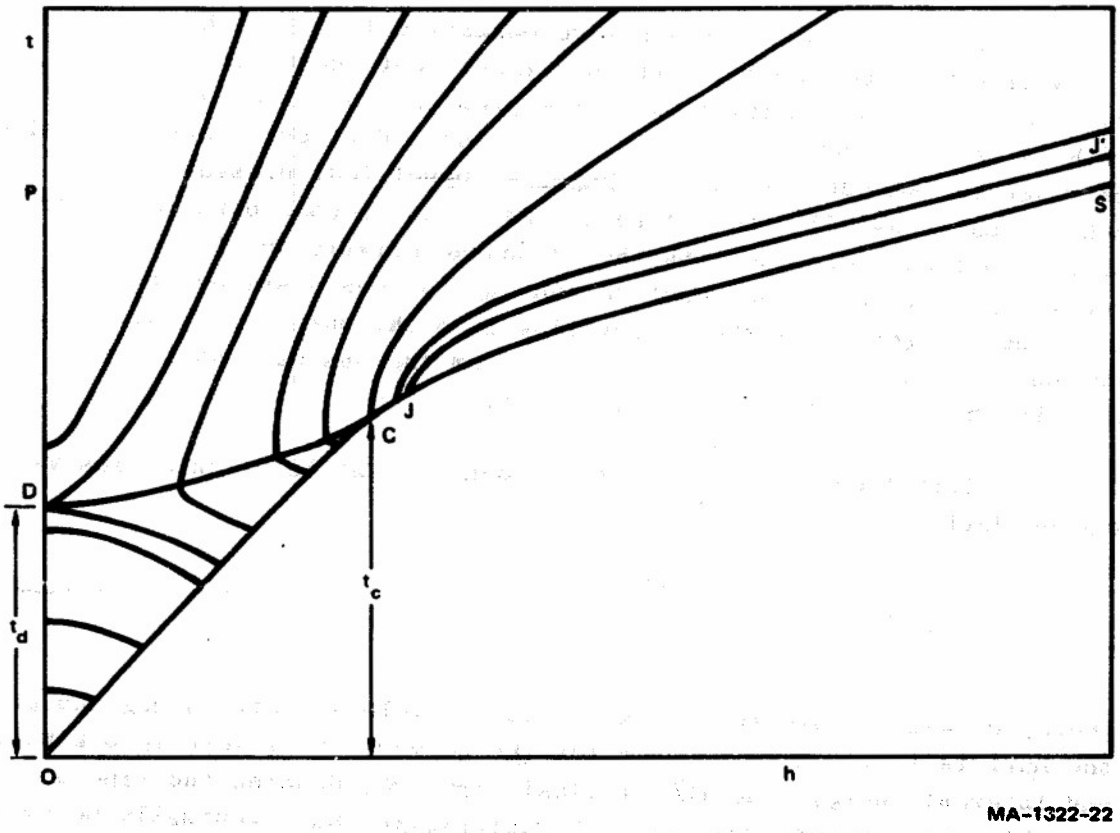

FIGURE 2 SCHEMATIC DIAGRAM OF THE LINES OF CONSTANT PRESSURE FOR THE INITIATION OF DETONATION UNITS $(\partial p/\partial h) > 0$

Consider now the locus of peaks DC where $\partial p/\partial t = 0$ and $Dp/Dt > 0$. Since

$$\frac{Dp}{Dt} = \frac{\partial p}{\partial h}\frac{Dh}{Dt} \qquad (105)$$

along DC, the slope of DC must be positive except at the double point, where it must be zero. Moreover since $\partial p/\partial h > 0$, it follows that $C_p = 0$ along CD for $t > t_d$ and consequently the curves of constant pressure intersecting CD are tangent to the particle paths as shown in Figure 2.

The curves of constant pressure emanating from the shock path after t_c will now be considered. It is evident that these curves cannot intersect the shock path again because the pressure increases along the shock path as the wave develops into a detonation. Particular attention should be given to the curve with the Chapman-Jouguet (CJ) pressure shown schematically as JJ' in Figure 2. JJ' must become parallel to the shock front and coincide with the CJ characteristic and the line of complete reaction as the reaction zone approaches a steady state. It consequently separates the steady flow from the unsteady flow, and all curves of constant pressure emanating from the unsteady shock above J must become parallel to the shock front.

A critical energy E_c for the shock initiation of an explosive can be defined as

$$E_c = \tfrac{1}{2}\int_0^{\alpha} pu\,dt \qquad (106)$$

where p and u are the pressure and particle velocity along the piston, the half is included to account for the conversion of work into kinetic and internal energy, and the critical time, α, denotes the time of formation of the forward-facing characteristic that eventually becomes the CJ characteristic in the steady detonation wave. Note that the critical energy is defined as a change in the internal energy rather than as the change in total energy specified by Walker and Wasley.[15] Since former work on initiation[16] suggests that this critical characteristic lies in a centered reactive rarefaction fan, α can in principle be determined by finding the position on the piston path where the second derivative of the characteristic becomes zero. Let s_+ denote the slope of a forward-facing characteristic, so that

$$s_+ = \frac{c}{(\partial r/\partial h)} = \frac{v_0 c}{v} \qquad (107)$$

The condition determining α can then be written as

$$\frac{ds_+}{dt} = v_0\left(\frac{\partial c/v}{\partial t} + s_+ \frac{\partial c/v}{\partial h}\right) = 0 \; . \tag{108}$$

Attempts were made to calculate p, u, and α along the piston to determine E_c for a polytropic medium with a simple reaction rate law but, since approximations must be made unless a complete solution to the reactive flow problem is known, a simpler approach to the critical energy problem was undertaken.

The alternative approach was to apply Eq. (106) to the steady state wave and assume that the amount of energy required to initiate a steady detonation with no delay time[17] is sufficient to initiate the explosive subjected to other initial conditions. Another way to look at this assumption is to say that, if there is a critical energy for initiation, its value will be determined by the properties of the steady state wave. Since the centered rarefaction fan in a steady wave emanates from the CJ point, the critical time α in the steady wave is taken as the reaction time. Evaluating Eq. (106) for a steady state detonation wave leads to the following equation for the critical energy

$$E_c = \frac{\rho_0 D^2 Z}{2} \frac{\langle[1 - \rho_0/\rho]\rangle}{\langle\rho_0/\rho\rangle} \tag{109}$$

where D denotes the detonation velocity, Z denotes the reaction zone length, and the density terms in brackets denote values averaged over the reaction zone. Equation (109) for the critical energy takes into account the initial state and the equation of state of the unreacted explosive, the equation of state of the reactive mixture, and the kinetics and thermochemistry of the exothermic reaction supporting detonation. However, it gives values larger than those determined experimentally by Walker and Wasley. This disparity suggests that calculations of critical energy with the steady state wave must account for the fact that the completion of reaction on the rear boundary is not a necessary condition for initiation of detonation.

VI THE REACTIVE SHOCK PROBLEM

Work was continued on the reactive shock problem with a prescribed energy release rate. Solutions for buildup to detonation were sought to provide a means of demonstrating the dependence of initiation on the energy release rate and on the rear-boundary conditions, and a means of calculating the critical energy for initiation defined in Section V. The new methods tried for constructing solutions for reactive shocks were unsuccessful however.

It is convenient to write the flow equations in terms of the Lagrange time τ introduced earlier in this report as

$$\frac{\partial v}{\partial t} = \frac{v_0}{U}\frac{\partial u}{\partial \tau} \tag{110}$$

$$\frac{\partial u}{\partial t} = -\frac{v_0}{U}\frac{\partial p}{\partial \tau} \tag{111}$$

$$\frac{\partial p}{\partial t} = -\left(\frac{c}{v}\right)^2 \frac{\partial v}{\partial t} + \frac{\Gamma}{v} q \frac{\partial \lambda}{\partial t} \; . \tag{112}$$

Our problem for a prescribed energy release rate is to find the volume field $v(t,\tau)$, the particle velocity field $u = u(t,\tau)$, and the pressure field $p(t,\tau)$, that satisfy the differential equations (110)-(112) along particle paths and satisfy the Rankine-Hugoniot jump conditions along the shock path where $t = \tau$. Previous attempts to solve this problem,[4] with the explosive described by Eq. (23), and the energy equation written as

$$\frac{\partial r}{\partial \tau}\frac{\partial p}{\partial t} = -\kappa p \frac{\partial u}{\partial \tau} + \frac{(\kappa - 1)^2}{2} \rho_H u_H(\tau)\dot{Q} \tag{113}$$

made use of the fact that the $v(t,\tau)$, $u(t,\tau)$, and $p(t,\tau)$ fields can be obtained from either the particle velocity gradient or the pressure gradient by integrating Eq. (38), Eq. (110), and Eq. (111) when the energy release rate at the shock front is prescribed. Consider, for example,

the case when the form of $\partial u/\partial\tau$ is assumed. Integration of Eq. (38) gives the shock pressure, the shock particle velocity follows from Eq. (37), and the shock path can then be obtained by integrating Eq. (35). Integration of Eq. (10) along a particle path from the shock front gives the volume field, and integration of $\partial u/\partial\tau$ and Eq. (111) along an isochrone from the shock path gives the corresponding particle velocity and pressure fields. Since the energy equation was not used, however, a solution for a reactive shock is obtained only if the assumed form of $\partial u/\partial\tau$ is compatible with the energy release rate and the calculated flow satisfies Eq. (113). A similar argument applies also to the case when the form of $\partial p/\partial\tau$ is assumed. The problem can therefore be regarded as that of finding the particle velocity gradient that is compatible with the prescribed energy release rate. This approach is practically intractable, however, because the flow is related to the reaction through the energy equation, and there is no apparent way that this equation can be used to determine the particle velocity gradient.

Since buildup to detonation is of particular interest, most attention was given to the final attainment of steady state flow. In one approach, the equations of motion were transformed so that their integrals consist of steady state terms and unsteady state terms that vanish as the steady state is attained. The independent variables were changed from (τ,t) to $(\tau,\xi = \tau - t)$ so that the partial derivatives transform as follows

$$\frac{\partial}{\partial\tau_t} \rightarrow \frac{\partial}{\partial\xi_\tau} + \frac{\partial}{\partial\tau_\xi} \tag{114}$$

$$\frac{\partial}{\partial t_\tau} \rightarrow - \frac{\partial}{\partial\xi_\tau} \tag{115}$$

and Eqs. (110) and (111) become

$$U\frac{\partial v}{\partial\xi} + v_o\frac{\partial u}{\partial\xi} = - v_o\frac{\partial u}{\partial\tau_\xi} \tag{116}$$

and

$$v_o\frac{\partial p}{\partial\xi} - U\frac{\partial u}{\partial\xi} = - v_o\frac{\partial p}{\partial\tau_\xi} \; . \tag{117}$$

Formal integration of Eqs. (116) and (117) with respect to ξ gives the equations expressing the conservation of mass and momentum for unsteady flow as

$$Uv = v_0(U - u) - v_0\int_0^{\xi} \left(\frac{\partial u}{\partial \tau}\right)_{\xi} d\xi \qquad (118)$$

$$p - p_0 = \rho_0 U u - \int_0^{\xi} \left(\frac{\partial p}{\partial \tau}\right)_{\xi} d\xi \qquad (119)$$

The corresponding equation for the energy is most conveniently derived by integrating the first law of thermodynamics written as

$$\frac{\partial e}{\partial \xi} + \frac{\partial pv}{\partial \xi} = v\,\frac{\partial p}{\partial \xi}\,. \qquad (120)$$

The combination of Eqs. (120), (117), and (118) leads to the equation

$$\frac{\partial e}{\partial \xi} + \frac{\partial pv}{\partial \xi} + (u - U)\frac{\partial u}{\partial \xi} = u\,\frac{\partial u}{\partial \tau}_{\xi} - v\,\frac{\partial p}{\partial \tau}_{\xi} - \frac{\partial u}{\partial \xi}\int_0^{\xi} \left(\frac{\partial u}{\partial \tau}\right)_{\xi} d\xi \qquad (121)$$

which can readily be integrated to give the equation expressing the conservation of mass, momentum, and energy as

$$e - e_0 + pv - p_0 v_0 + \tfrac{1}{2}(u - U)^2 - \tfrac{1}{2}U^2 = \int_0^{\xi}\left[u\left(\frac{\partial u}{\partial \tau}\right)_{\xi} - v\left(\frac{\partial p}{\partial \tau}\right)_{\xi}\right]d\xi - u\int_0^{\xi}\left(\frac{\partial u}{\partial \tau}\right)_{\xi} d\xi\,. \qquad (122)$$

Equations (118), (119), and (122) can be regarded as perturbed Rankine-Hugoniot equations because they reduced to these equations as the flow attains a steady state and the derivatives $(\partial u/\partial \tau)_{\xi} = 0$ and $(\partial p/\partial \tau)_{\xi}$ becomes zero. Attempts to use these equations in a perturbation analysis to construct solutions for the final approach to the steady state were unsuccessful.

In the second approach to the reactive shock problem, the energy equation was integrated rather than used as a compatibility condition as in the previous treatment.[4] Although the pressure and volume fields generated from the energy equation are compatible with a prescribed energy release rate, there is no guarantee that they are associated

with a unique particle velocity field because the continuity and momentum equations were not used in their construction. The continuity and momentum equations were therefore combined to obtain a condition that the pressure and volume must satisfy in order to be a solution to a reactive shock problem. This compatibility condition was derived as

$$-u_H \frac{du_H}{d\tau} \frac{\partial p}{\partial \tau} + p_H^2 \frac{\partial^2 v}{\partial t^2} = -u_H^2 \frac{\partial^2 p}{\partial \tau^2} \tag{123}$$

by eliminating $\partial^2 u/\partial t \partial \tau$ from the equations obtained by differentiating Eq. (110) partially with respect to t and differentiating Eq. (111) partially with respect to τ.

A simple case was considered first. An expression relating the volume and reaction was chosen as

$$\frac{v}{v_H} = \frac{(\partial r/\partial \tau)}{(\partial r/\partial \tau)_H} = G(\lambda) \tag{124}$$

so that the energy equation could be integrated without difficulty, and the reaction was assumed to have no activation energy. The reaction rate was written formally as

$$\frac{\partial \lambda}{\partial t} = \frac{1}{\alpha} R(1 - \lambda) \tag{125}$$

with $R(1) = 1$ and $R(0) = 0$, so that $\partial\lambda/\partial t = -\partial\lambda/\partial\tau$ and the reaction rate at the shock front is constant. Integration of the energy equation gives the equation for the pressure field as

$$p - p_H(\tau) = \frac{(\kappa + 1)p_D}{4(\kappa - 1)G(\lambda)}[F(\lambda) - F(0)] \tag{126}$$

where p_D denotes the spike pressure in a CJ wave and F is defined by the equation $dF/d\lambda = G^{\kappa-1}$. Integration of the differential equation along the shock path gives the equation for the shock pressure as

$$p_h(t) = (p_i - P_D) \exp\left(-\frac{(\kappa + 1)}{3} g(0)t/\alpha\right) + P_D \tag{127}$$

where $P_D = p_D/2(\kappa - 1)g(0)$, $g(0) = \alpha(\partial u/\partial r)_H = (d\ \ln G/d\lambda)_H$, and p_i denotes the initial shock pressure $t = 0$. Examination of conditions for buildup to a steady state gives G as

$$(\kappa - 1)G = \kappa - (1 - \lambda)^{\frac{1}{2}} \tag{128}$$

and the equations for $g(0)$ and F are obtained from Eq. (128) as

$$2(\kappa - 1)\ g(0) = 1 \tag{129}$$

$$F(\lambda) - F(0) = \frac{2(\kappa - 1)}{(\kappa + 1)} [G^{\kappa}(1 + (1 - \lambda)^{\frac{1}{2}} - 2] \tag{130}$$

Equations (126) and (127) then give the equations for the pressure field as

$$p = \frac{p_D}{2} (1 + (1 - \lambda)^{\frac{1}{2}}) + \frac{p_H(\tau) - p_D}{G^{\kappa}} \tag{131}$$

$$p_H(\tau) = \left(p_i - p_D\right)\exp\left[-\frac{(\kappa + 1)}{6(\kappa - 1)}\frac{t}{\alpha}\right] + p_D . \tag{132}$$

The fact that Eqs. (124), (131), and (132) do not satisfy Eq. (123) leads to the conclusion that Eq. (124) cannot be satisfied in a time-dependent wave that builds up to a steady state. In other words, Eq. (124) is too restrictive and must be generalized to obtain a more realistic treatment of unsteady flow.

Other attempts to construct solutions for the final stages of initiation were based on the assumption that the fall in pressure along a particle path is proportional to the fall in pressure along a particle path in the steady state wave. The equation expressing this condition is obtained from the equation for the pressure in a CJ wave $p = p_D/2(1 + (1 - \lambda^{\frac{1}{2}})$ as

$$\frac{\partial p}{\partial t} = -\frac{p_D E}{4(1 - \lambda)^{\frac{1}{2}}} \frac{\partial \lambda}{\partial t} \tag{133}$$

with E an arbitrary function of τ. A unimolecular reaction with no activation energy was considered to simplify the integration of the energy equation. In this case, Eq. (133) reduces to the equation

$$\frac{\partial p}{\partial t} = -\frac{p_D}{4\alpha} E(\tau) e^{\frac{\tau - t}{2\alpha}} \tag{134}$$

since $1 - \lambda = e^{(\tau-t)/\alpha}$. Integration of Eq. (134) gives the equation for the pressure field, which is written for convenience as

$$p = \frac{p_D}{2}\left(B + E e^{\frac{\tau-t}{2\alpha}}\right) \tag{135}$$

with B another arbitrary function of τ. Integration of the energy equation gives the corresponding volume field as

$$v = \frac{v_0}{(\kappa + 1)E^2}\left(\kappa B - E e^{\frac{\tau-t}{2\alpha}}\right). \tag{136}$$

Evaluating Eq. (136) at the shock front, however, where $v = v_D = [(\kappa - 1)/(\kappa + 1)]v_0$ and $t = \tau$ gives the following relationship between E and B,

$$\kappa B = (\kappa - 1)E^2 + E . \tag{137}$$

The equations for the pressure and volume can therefore be written in terms of the arbitrary function E as

$$p = \frac{p_D}{2}\left[\frac{(\kappa - 1)E^2}{\kappa} + E\left(\frac{1}{\kappa} + e^{\frac{\tau-t}{2\alpha}}\right)\right] \tag{138}$$

and

$$v = \frac{v_0}{(\kappa + 1)}\left[(\kappa - 1) + \frac{1}{E}\left(1 - e^{\frac{\tau-t}{2\alpha}}\right)\right]. \tag{139}$$

The equation for the shock pressure follows from (138) as

$$p_H = \frac{p_D}{2\kappa}\left((\kappa - 1)E^2 + (\kappa + 1)E\right) \tag{140}$$

and the differential equation for shock pressure leads to the following

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equation for E

$$\frac{dE}{d\tau} = \frac{(1 - E)}{6\alpha\left(1 + [(\kappa - 1)/(\kappa + 1)]E\right)} \ . \qquad (141)$$

The question now arises whether Eqs. (138) and (139) satisfy the compatibility condition. The equations obtained by differentiating Eqs. (138) and (139), together with Eq. (141), show that Eq. (123) is not satisfied. Here again the assumption made about the flow was not realistic enough and we were unable to find a solution for the final buildup to detonation.

VII RESULTS AND RECOMMENDATIONS

The results of the theoretical study of reactive shock waves presented in this report lead to a better understanding of the initiation of detonation in condensed explosives.

Various aspects of shock initiation were considered. The differential equation governing a shock discontinuity was used to determine different conditions for a single shock trajectory for buildup to detonation. One of these conditions for single shock buildup produced by a flying plate was used to construct a solution for the type of flow observed by Kennedy[10] during the early stages of initiation in PBX 9404.

Other properties of initiation induced by a constant velocity piston or a flying plate were considered. The equations relating the initial flow to the initial energy release rate in such a wave were derived. These equations provide a means of determining the variation of energy release rate with pressure at the front of the wave when the Hugoniot curve of the explosive is known. Conditions were also determined for the shock produced by a constant velocity piston to accelerate with either a positive or a negative pressure gradient. These conditions are important because they demonstrate how the mechanism of initiation depends on the energy release rate, the sound speed, and the relationship between these quantities. A critical energy for initiation was defined for the case when the wave builds up with a positive pressure gradient. Work on the reactive shock problem was continued, and integral relationships for unsteady flow were derived as generalized Rankine-Hugoniot equations without making approximations. Attempts to construct explicit solutions for the initiation of steady state waves so that critical energies could be calculated were however unsuccessful.

Steady state detonation was considered, and a perturbation analysis for a simple reaction was carried out to determine a sufficient condition for its stability.

Additional studies that would extend the work presented in this report are recommended to improve our present understanding of the initiation of detonation in condensed explosives. A general criticality

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Appendix

STABILITY OF THE STEADY DETONATION

An objective of the research reported here has been to separate initial conditions leading to steady detonation from those producing extinction or some sort of irregular burning. For initial conditions close to the steady state, the problem is one of finding the stability boundary where perturbations in parameter values on one side of the boundary lead to steady detonation while those on the other side do not.

A first attempt at locating the stability boundary is made below by examining whether a small initial irregularity will grow. The irregularity at a point in the unburnt material is swept over by the shock. The perturbation wave in the reacting flow behind the shock is headed by a sound wave or characteristic. It is found that the effect of the initial disturbance dies away along the characteristic if κ, the polytropic index, is small enough; the critical κ depends on n, the order of the reaction. If κ is larger than this value, the initial disturbance does increase with time, at least part way along the characteristic, so that an instability can arise. The results is sketched for a particular case in Figure A-1.

Steady State

The gas dynamic equations for one-dimensional, adiabatic, reactive flow read

$$\dot{\rho} + \rho u_x = 0$$

$$\rho\dot{u} + p_x = 0$$

$$\dot{p} + \kappa p u_x = (\kappa - 1)Q\rho R$$

$$\dot{\lambda} = R$$

where ρ is the gas density, p the pressure, u the particle velocity, λ the fraction of gas reacted at rate R, κ the polytropic

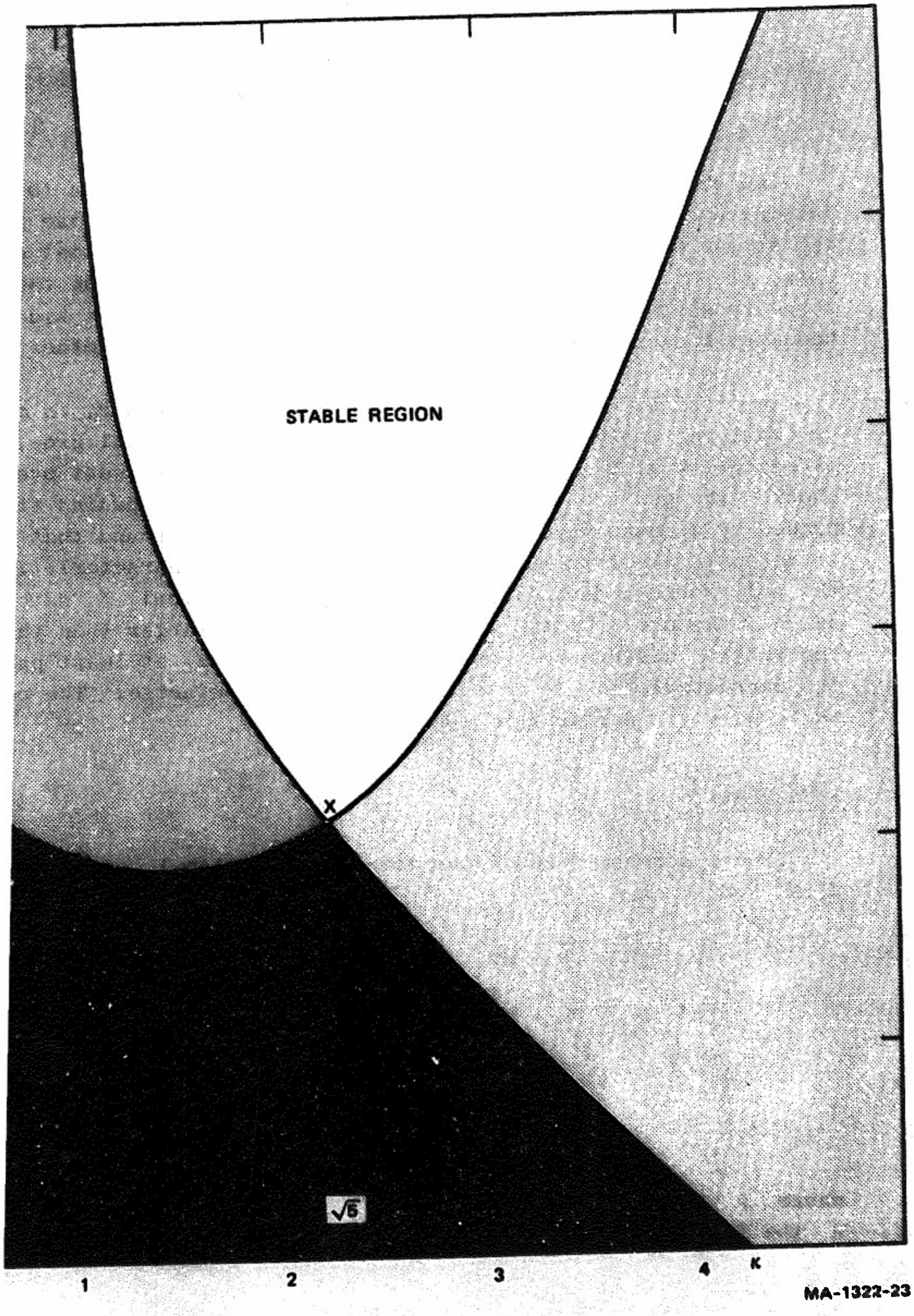

FIGURE A-1 STABLE REGION IN PARAMETER PLANE

index, and Q the heat released. The Eulerian coordinates are distance x and time t with the superior dot denoting the material time derivative.

Solutions of the equations representing steady states are those where ρ, p, u, and λ are functions of $(t - x/D)$ only, where D is a constant speed. If the steady state is headed by a strong shock moving at speed D into quiescent gas of density ρ_0, the jump conditions give just behind the shock

$$u = 2D/(\kappa + 1)$$

$$\rho = \rho_0 (\kappa + 1)/(\kappa - 1)$$

$$p = \rho D u$$

$$\lambda = 0$$

The corresponding steady state is

$$\rho = \rho_0 D/(D - u)$$

$$p = \rho_0 D u$$

$$\lambda = u[D - (\kappa + 1)\, u/2]/(\kappa - 1)Q$$

The Chapman-Jouguet condition, that $D = u + c$ where the reaction is complete $(\lambda = 1)$, is satisfied if

$$D^2 = 2(\kappa^2 - 1)Q$$

Here c is the sound speed given by

$$c^2 = \kappa u(D - u)$$

The above steady state equations relate the dependent variables to one another. Their relation to the coordinate locations is found from the reaction equation

$$\dot{\lambda} = R$$

This equation can be expanded to read

$$2(\kappa + 1)(D - u)[D - (\kappa + 1)u]u'/D^3 = R$$

where the prime denotes differentiation with respect to $(t - x/D)$. Integration gives

$$t - x/D \;=\; \int^{u} 2(\kappa + 1)(D - u)[D - (\kappa + 1)u]du/D^3R$$

The particular form for R used below is

$$R \;=\; \rho^{n-1}(1 - \lambda)^{n}/\alpha$$

where α and n are constants. This form approximates the rate expression for a reaction of order n with simple pressure dependence. Since

$$1 - \lambda \;=\; [D - (\kappa + 1)u]^2/D^2$$

one sees that this reaction is complete in a finite time only if $n < 1$.

Perturbation Equations

For a small perturbation of the steady state,

$$\rho \;=\; \bar{\rho} + \epsilon\tilde{\rho}, \qquad u \;=\; \bar{u} + \epsilon\tilde{u}, \qquad \text{etc.},$$

where the bar indicates the steady state function given above, the tilde denotes a quantity of ordinary magnitude, and ϵ is a small constant. Substitution in the gas dynamic equations gives, to the first order in ϵ,

$$\rho_t + \bar{u}\rho_x + u\bar{\rho}_x + \rho\bar{u}_x + \bar{\rho}u_x \;=\; 0$$

$$\rho(\bar{u}_t + \bar{u}\bar{u}_x) + \bar{\rho}(u_t + \bar{u}u_x + u\bar{u}_x) + p_x \;=\; 0$$

$$p_t + \bar{u}p_x + u\bar{p}_x + \kappa(\bar{p}u_x + p\bar{u}_x) \;=\; (\kappa - 1)\,Q(\bar{\rho}R + \rho\bar{R})$$

$$\lambda_t + \bar{u}\lambda_x + u\bar{\lambda}_x \;=\; R$$

where the tildes have been omitted from the perturbation quantities for simplicity.

Along particle paths, linear combinations of the equations in characteristic form read:

$$\lambda_t + \bar{u}\lambda_x + u\bar{\lambda}_x = R$$

$$-\bar{c}^2(\rho_t + \bar{u}\rho_x) + p_t + \bar{u}p_x - \bar{c}^2(u\bar{\rho}_x + \rho\bar{u}_x) + \bar{p}_x u + \kappa p\bar{u}_x$$

$$= (\kappa - 1)Q(\bar{\rho}R + \rho\bar{R})$$

along particle paths, and

$$p_t + (\bar{u} \pm \bar{c})p_x \pm \bar{c}\bar{\rho}[u_t + (\bar{u} \pm \bar{c})u_x]$$

$$\pm \bar{c}(\rho[\bar{u}_t + \bar{u}\bar{u}_x] + \bar{\rho}\bar{u}_x u) + \bar{p}_x u + \kappa p\bar{u}_x$$

$$= (\kappa - 1)Q(\bar{\rho}R + \rho\bar{R})$$

along forward (+) and backward (-) sound waves.

The perturbation at the shock is found in the same way:

$$\tilde{u} = 2\tilde{D}/(\kappa + 1)$$

$$\tilde{\rho} = 0$$

$$\tilde{p} = 2\bar{\rho}\bar{D}\tilde{u}$$

$$\tilde{\lambda} = 0$$

Irregularity at a Point

A small irregularity is supposed present at a point in the unburnt material. When the shock reaches this point it will experience a velocity perturbation $\epsilon\tilde{D}$. Corresponding perturbations $\tilde{u}$, $\tilde{\rho}$, $\tilde{p}$, and $\tilde{\lambda}$ arise according to the shock equations given above. The expressions are made precise by setting $\tilde{D} = 1$ and putting the magnitude of the perturbation into ϵ. The only requirement is that ϵ is small enough that it is reasonable to neglect ϵ with respect to 1.

The first effect of the irregularity is a discontinuity propagated along the backward running sound wave. Since particle paths cross this sound wave, the equation

$$\lambda_t + \bar{u}\lambda_x + u\bar{\lambda}_x = R$$

holds across the wave in spite of the jump in the value of u and perhaps of R. One sees that the equation remains satisfied by an abrupt change in the cross-derivative of λ,

$$\lambda_t + \bar{u}\lambda_x$$

if needed, and not by any change in λ itself. The perturbation λ therefore retains just behind the sound wave the value zero that it had in the steady flow ahead of the wave. On the wave

$$\lambda = 0$$

The other equation valid along particle paths may be written

$$(p - \bar{c}^2 \rho)_t + \bar{u}(p - \bar{c}^2 \rho)_x + \rho(\bar{c}^2_t + \bar{u}\bar{c}^2_x) - \bar{c}^2 (u\bar{\rho}_x + \rho\bar{u}_x) + \bar{p}_x u + \kappa p\bar{u}_x$$

$$= (\kappa - 1)Q(\bar{\rho}R + \rho\bar{R})$$

By the same argument as above, one finds that

$$p - \bar{c}^2 \rho = 0$$

on the sound wave.

From the forward running sound wave in the same way,

$$p + \bar{\rho}\bar{c}u = 0$$

The above relations valid along the backward running sound wave permit the elimination of p, ρ, and λ from the equation for the wave. One obtains

$$u_t + (\bar{u} - \bar{c})u_x + (\bar{u}'/4\kappa\bar{c}\bar{D}\bar{u})Mu = 0$$

where

$$M = \kappa^2\bar{u}\bar{D} + \bar{c}[(\kappa - 2)\bar{D} + 2(1 - \kappa^2)\bar{u}] + [\kappa\bar{D}^3\bar{u}/(\kappa + 1)\bar{u}'](\tilde{R}/\tilde{u})$$

Since $\bar{u}'$ has the same sign as R, which is positive, the coefficient of Mu in the differential equation is positive. One sees that the perturbation at the shock grows with time along the sound wave

if M is negative and decays if M is positive. Since M varies with $\bar{u}$, decay and therefore stability are assured only if M is positive for the whole range of values of $\bar{u}$. This stability criterion is examined for a particular rate expression below.

Stability of a Particular Reaction

For the reaction

$$R = \rho^{n-1}(1 - \lambda)^n/\alpha$$

one finds

$$\tilde{R}/\bar{R} = (n - 1)(\tilde{\rho}/\bar{\rho}) - n\tilde{\lambda}/(1 - \bar{\lambda})$$

Since along the backward running sound wave propagated from the initial disturbance

$$\tilde{\lambda} = 0$$

and

$$\tilde{\rho} = (\bar{\rho}/\bar{c})\tilde{u}$$

one finds

$$\tilde{R}/\tilde{u} = (n - 1)\bar{R}/\bar{c}$$

Use of the expressions for these steady state quantities in terms of $\bar{u}$ gives finally

$$M = \kappa^2\bar{u}\bar{D} + \bar{c}[(\kappa + n - 3)\bar{D} + (\kappa + 1)\bar{u}(3 - n - 2\kappa)]$$

An investigation of the equation of M for $\bar{u}$ on its range $\bar{D}/(\kappa + 1) \le \bar{u} \le 2\bar{D}/(\kappa + 1)$ is now required.

If one sets $M = 0$, one finds that there are generally three roots for $\bar{u}$. One of these roots is at the C-J value, $\bar{u} = \bar{D}/(\kappa + 1)$, for any values of κ and n. There is a second root at $\bar{u} = \bar{D}/(\kappa + 1)$ if

$$n = 3 + \kappa(\kappa - 3)$$

There is a root at the shock, $\bar{u} = 2\bar{D}/(\kappa + 1)$, if

$$n = 3 + \kappa\{-2 \pm [(\kappa + 1)/(\kappa - 1)]^{\frac{1}{2}}\}$$

These two curves cross at point E where $A = \xi^3$ and $B = (\frac{1}{2})(11 - 3(\xi)^{\frac{1}{2}})$. There are no roots for [illegible] in [illegible] and the sign of [illegible] is positive so that the steady state solution is stable for points in the quadrant between the curves and above point E, as shown in Figure C1. The remaining may be stable elsewhere but a deeper analysis involving the flow behind the initial characteristic is needed to prove it.

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